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Shape analysis of carbon nanotube junctions

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Abstract. Using the eigenvectors of the Laplacian matrix of the graph describing the topology of a nanotube junction we have developed a shape analysis. The **X**, **Y**, **Z** relaxed Descartes coordinates of the atoms were calculated as a linear combination of the eigenvectors. We found that the partial sums generated three-dimensional structures only if they contained all the three bi-lobal eigenvectors of the Laplacian. We obtained partial sums that produced satisfactory initial coordinates for molecular mechanics calculations.

Introduction

There are several theoretical proposals for various carbon nanotube junctions [1-21] and in most of the cases the position of the atoms are given with the help of a molecular mechanics procedure. It was found, however, that some eigenvectors of the adjacency matrix can produce satisfactory Descartes coordinates for several spherical, toroidal and planar structures [22-31]. In these procedures, it is supposed that the molecules of fullerenes are spherical, the tori can be imagined as the direct product of two circles. The topological coordinates of nanotubes and planar structures are developed from the correspondent topological coordinates of tori. The question arises whether the method of the topological coordinates can be used for non-spherical structures as well? Here we present a shape analysis of nanotube junctions in order to explore the possibility to extend the topological coordinate method to non-spherical structures.

Topological coordinates

The atomic arrangement of a molecule can be described by the graph $G = (V, E)$ where V is the set of vertices and E is that of the edges. Let $A = (a)$ be the adjacency matrix of the graph G on n vertices. The vertices i, j are understood to be adjacent if $a_{ij} = 1$. For non-adjacent vertices $a_{ij} = 0$. The vertices correspond to the carbon atoms and the edges to the first neighbour bonds. Let the diagonal matrix D be given by $d_{ii} = d(i)$, where $d(i)$ is the degree of a vertex i. The Laplacian matrix $\mathbf{L}$ is defined as $\mathbf{L} = \mathbf{A} - \mathbf{D}$. This definition of $\mathbf{L}$ correspond to the usual definition of the Laplacian if it is multiplied by -1. Using our definition, the ordering of the eigenvectors of the adjacency matrix and the Laplacian is the same. By the aid of A and L matrices, we can describe the topological structure but, for further investigation, usually we need the Cartesian coordinates of the atoms as well. A simple solution to this problem is to use the topological coordinate method proposed by Fowler and Manolopoulos [22] and by Pisanski and Shawe-Taylor [23]. The topological coordinate method is based on the so called bi-lobal eigenvectors of the adjacency matrix [22-25]. Eigenvectors having this bi-lobal property can be identified by the graph-disconnection test [26]: for a candidate eigenvector, colour all vertices of $G = (V, E)$ bearing positive coefficients black, all bearing negative coefficients white, and all having a zero coefficient grey; now delete all grey vertices, all edges connecting a black to a white vertex; if the graph now consists of exactly two connected components, one of black and one of white vertices, then the eigenvector is bi-lobal. If the number of connected uncoloured subsets is greater than two we call the correspondent eigenvector multi-lobal.

Arrange in descending order the $n = |V|$ eigenvalues λ_k of the adjacency matrix A as:

$$\lambda_1 > \lambda_2 \geq \lambda_3 \geq ... \geq \lambda_n \qquad (1)$$

where c_k is the eigenvector with eigenvalue λ_k. In the case of structures homeomorphic to the sphere, like fullerenes, the first three bi-lobal eigenvectors c_{k_1}, c_{k_2}, and c_{k_3} determine the (x_i, y_i, z_i) topological coordinates of the i-th atom by the relations:

$$x_i = S_1 c_{k_1 i} \qquad (2)$$

$$y_i = S_2 c_{k_2 i} \qquad (3)$$

$$z_i = S_3 c_{k_3 i} \qquad (4)$$

with the scaling factors $S_\mu = 1$ or $S_\mu = \frac{1}{\sqrt{\lambda_1 - \lambda_{k_\mu}}}$. The most realistic picture of fullerenes can be found by the the scaling factor: [22,27]

$$S_\mu = \frac{1}{\sqrt{\lambda_1 - \lambda_{k_\mu}}} \quad . \qquad (5).$$

In the last years, the topological coordinate method was extended to tori [26,28,29], nanotubes[27,29] and planar[30,31] structures.

The graph of a nanotube junction

By introducing two unit vectors $a_1 = a\begin{pmatrix}\sqrt{3}\\ 0\end{pmatrix}$ and $a_2 = a\begin{pmatrix}\sqrt{3}/2\\ 3/2\end{pmatrix}$ on the graphene sheet and two integers k and l we can assign coordinates (k,l) to each hexagon of the sheet [32]. Hexagonal nanotubes are obtained by rolling up a rectangle defined by the chiral vector

$$\mathbf{C}_h = m\mathbf{a_1} + n\mathbf{a_2} \qquad (6)$$

and the multiple of the translation vector

$$T = [-(2n+m)a_1, (2m+n)a_2]/d_R \qquad (7)$$

where m and n are integers and d is the highest common divisor of (m,n), with $d_R = d$ if $n - m$ is not a multiple of $3d$. During the rolling up procedure the sides parallel to the translation vector T are identified [32].

Let us suppose that we want to calculate the topological coordinates of a junction made of three open ended nanotubes with (m,n) parameters $(9,6)$, $(8,7)$ and $(10,5)$. We suppose further that the topological structure of the junction is constructed by some algorithm as for example of references [1-21]. That is, we know the graph $G = (V,E)$ of the junction. In our particular case, the number of vertices and edges are in order $|V| = 1165$ and $|E| = 1723$.

The atomic coordinates are in Angstroms and the interatomic distances are about 1.4 Å.

Shape analysis of nanotube junctions

The eigenvectors of the adjacency matrix A provide improper topological coordinates for a nanotube junction by applying Eqs (1-5).

There are two problems with the obtained structures. The first one is that the ends of the nanotubes turn back and the second one is they become narrower as one moves to their tips. We could eliminate the first problem by replacing the adjacency matrix A by the Laplacian L. In order to find information for the second problem, we performed a shape analysis based on the eigenvectors of the Laplacian.

Let us suppose we have the exact (x_i, y_i, z_i) coordinates of the atoms in the nanotube junction. In this case, **X, Y** and **Z** are n-dimensional vectors containing the x, y and z coordinates of the atoms, in order. We suppose that the centre of mass of the molecule is in the origin and the molecule is directed in such a way that the eigenvectors of its tensor of inertia show the directions of the x, y and z axes.

Using the following scalar products:

$$\alpha_{Xk} = \mathbf{X}\mathbf{c}_k, \quad \alpha_{Yk} = \mathbf{Y}\mathbf{c}_k \text{ and } \quad \alpha_{Zk} = \mathbf{Z}\mathbf{c}_k \tag{10}$$

the atomic coordinates can be written as

$$\mathbf{X} = \sum_{k=1}^{n} \alpha_{Xk} \mathbf{c}^k, \quad \mathbf{Y} = \sum_{k=1}^{n} \alpha_{Yk} \mathbf{c}^k \quad \text{and} \quad \mathbf{Z} = \sum_{k=1}^{n} \alpha_{Zk} \mathbf{c}_k. \tag{11}$$

Here $\mathbf{c}_k$ is the eigenvector of the Laplacian L and the corresponding eigenvectors λ_k are ordered in descending order, as in Eq. (1). The weight of the eigenvector $\mathbf{c}_k$ in **X** is $|\alpha_{Xk}|^2$. We use similar notation for $|\alpha_{Yk}|^2$ and $|\alpha_{Zk}|^2$, corresponding to the weight of $\mathbf{c}_k$ in **Y** and **Z**.

Table 1. shows the calculated α_{Xk}, α_{Yk} and α_{Zk} coefficients for the structure under study. The junction of three nanotubes $(9,6)$, $(8,7)$ and $(10,5)$ contains 1165 vertices and 1723 edges while the atomic coordinates are in Angstroms, with interatomic distance about 1.4 Å.

The lobality of the 50 highest eigenvalues of the Laplacian is shown in Table 2.

Let we introduce the notations

$$\mathbf{X}_i^{(m)} = \sum_{k=1}^{m} \alpha_{Xk} \mathbf{c}_i^k, \quad \mathbf{Y}_i^{(m)} = \sum_{k=1}^{m} \alpha_{Yk} \mathbf{c}_i^k \text{ and } \quad \mathbf{Z}_i^{(m)} = \sum_{k=1}^{m} \alpha_{Zk} \mathbf{c}_i^k \tag{12}$$

and

$$R = (X, Y, Z), \qquad R^{(m)} = \left(X^{(m)}, Y^{(m)}, Z^{(m)}\right). \tag{13}$$

The convergence of the structure can be quantified by the following parameters:

$$\left|X - X^{(m)}\right| = \frac{1}{n}\left(\sum_{i=1}^{n}\left(X_i - X_i^{(m)}\right)^2\right)^{\frac{1}{2}} \tag{14}$$

$$\left|Y - Y^{(m)}\right| = \frac{1}{n}\left(\sum_{i=1}^{n}\left(Y_i - Y_i^{(m)}\right)^2\right)^{\frac{1}{2}} \tag{15}$$

$$\left|Z - Z^{(m)}\right| = \frac{1}{n}\left(\sum_{i=1}^{n}\left(Z_i - Z_i^{(m)}\right)^2\right)^{\frac{1}{2}} \tag{16}$$

$$\left|R - R^{(m)}\right| = \frac{1}{n}\sum_{i=1}^{n}\left(\left(X_i - X_i^{(m)}\right)^2 + \left(Y - Y_i^{(m)}\right)^2 + \left(Z - Z_i^{(m)}\right)^2\right)^{\frac{1}{2}} \tag{17}$$

Table 3. shows these parameters calculated for our nanotube junction.

Table 1. The α_{Xk}, α_{Yk} and α_{Zk} coefficients in the function of the k<51 eigenvectors of the graph under study.

k	α	α	α
1.0000000	0.0000000	0.0000000	0.0000000
2.0000000	531.5254607	13.3827301	0.6325792
3.0000000	-16.2079966	430.8542357	0.0952077
4.0000000	3.5449696	-13.0315564	-5.4410281
5.0000000	42.4655249	-2.8137039	-9.6967041
6.0000000	2.0122291	27.8030055	-4.3774035
7.0000000	1.4159249	-2.0932022	-116.3577655
8.0000000	3.1082390	-70.5642098	9.2422098
9.0000000	-50.0196729	18.0156682	4.3182771
10.0000000	25.0383045	9.8005451	5.8380187
11.0000000	-51.9100731	-6.4189166	-2.6698094
12.0000000	-6.9409825	-32.8224709	4.6656589
13.0000000	-9.9775458	-26.2444492	-12.8144739
14.0000000	0.9532447	1.4957518	39.5057271
15.0000000	14.5111931	1.2285586	2.3931973
16.0000000	-0.4005245	-24.0277980	0.3733706
17.0000000	-1.4364734	-0.6421640	-4.8800356
18.0000000	0.0620605	-2.1570805	2.0228203
19.0000000	-0.0290088	-0.3082656	5.7207245
20.0000000	-0.2273765	1.4636923	-0.4286804
21.0000000	-0.4610300	2.8193019	0.7213372
22.0000000	-0.6741517	-0.4142709	-9.9134401
23.0000000	1.3758623	5.7961101	-1.3705850
24.0000000	7.7266471	-0.3504044	-0.2477901
25.0000000	1.2064242	0.3481832	0.6712200
26.0000000	1.3092264	1.7305266	0.1196681
27.0000000	-2.7900128	0.6966942	3.4279522
28.0000000	7.1753631	-0.6887413	0.5888154
29.0000000	-8.0446988	-1.7900420	0.3661587
30.0000000	1.2894355	-6.3156190	1.1002530
31.0000000	-0.3864592	2.2830875	1.3178089

36	4	0	4	-0.2116284
37	5	0	4	-0.2169469
38	2	0	5	-0.2182420
39	3	0	4	-0.2207537
40	3	0	3	-0.2233979
41	3	0	6	-0.2254453
42	4	0	3	-0.2272445
43	3	0	5	-0.2386275
44	2	0	5	-0.2407462
45	2	0	5	-0.2421679
46	4	0	4	-0.2439944
47	5	0	6	-0.2470364
48	2	0	8	-0.2550913
49	7	0	2	-0.2557325
50	6	0	3	-0.2612426

Table 3. The measure of convergences $\left|R - R^{(m)}\right|$, $\left|X - X^{(m)}\right|$, $\left|Y - Y^{(m)}\right|$ and $\left|Z - Z^{(m)}\right|$ in the function of m. Here m is the number of eigenfunctions used in the summation.

m	$\left\|R - R^{(m)}\right\|$	$\left\|X - X^{(m)}\right\|$	$\left\|Y - Y^{(m)}\right\|$	$\left\|Z - Z^{(m)}\right\|$
1.00000	18.89260	0.46309	0.37880	0.10781
2.00000	11.76644	0.07931	0.37863	0.10781
3.00000	5.24199	0.07808	0.08113	0.10781
4.00000	5.22797	0.07802	0.08035	0.10771
5.00000	5.09352	0.06898	0.08031	0.10739
6.00000	5.05286	0.06896	0.07669	0.10732
7.00000	3.55927	0.06895	0.07667	0.03928
8.00000	2.87028	0.06890	0.04700	0.03847
9.00000	2.48959	0.05388	0.04438	0.03829
10.00000	2.36666	0.04941	0.04358	0.03796
11.00000	1.89116	0.02136	0.04323	0.03789
12.00000	1.64505	0.02051	0.03278	0.03768
13.00000	1.45780	0.01864	0.02382	0.03603
14.00000	1.00749	0.01862	0.02378	0.01219
15.00000	0.91779	0.01384	0.02376	0.01201
16.00000	0.66298	0.01383	0.01180	0.01201
17.00000	0.64758	0.01378	0.01178	0.01126
18.00000	0.64253	0.01378	0.01164	0.01112
19.00000	0.61875	0.01378	0.01163	0.00998
20.00000	0.61776	0.01378	0.01157	0.00997
21.00000	0.61914	0.01377	0.01131	0.00995
22.00000	0.54523	0.01376	0.01131	0.00516
23.00000	0.52314	0.01371	0.01015	0.00503
24.00000	0.48155	0.01200	0.01015	0.00502
25.00000	0.48035	0.01195	0.01014	0.00499
26.00000	0.48050	0.01190	0.01003	0.00499
27.00000	0.46324	0.01166	0.01002	0.00403
28.00000	0.41534	0.00990	0.01000	0.00400
29.00000	0.36303	0.00709	0.00988	0.00398
30.00000	0.32434	0.00700	0.00826	0.00387
31.00000	0.31665	0.00700	0.00802	0.00370
32.00000	0.29962	0.00697	0.00734	0.00370
33.00000	0.29815	0.00696	0.00733	0.00363
34.00000	0.29762	0.00695	0.00731	0.00362
35.00000	0.29308	0.00684	0.00729	0.00362
36.00000	0.29182	0.00679	0.00729	0.00362
37.00000	0.28869	0.00679	0.00710	0.00362
38.00000	0.28152	0.00678	0.00682	0.00362

36	4	0	4	-0.2116284
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41	3	0	6	-0.2254453
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6.00000	5.05286	0.06896	0.07669	0.10732
7.00000	3.55927	0.06895	0.07667	0.03928
8.00000	2.87028	0.06890	0.04700	0.03847
9.00000	2.48959	0.05388	0.04438	0.03829
10.00000	2.36666	0.04941	0.04358	0.03796
11.00000	1.89116	0.02136	0.04323	0.03789
12.00000	1.64505	0.02051	0.03278	0.03768
13.00000	1.45780	0.01864	0.02382	0.03603
14.00000	1.00749	0.01862	0.02378	0.01219
15.00000	0.91779	0.01384	0.02376	0.01201
16.00000	0.66298	0.01383	0.01180	0.01201
17.00000	0.64758	0.01378	0.01178	0.01126
18.00000	0.64253	0.01378	0.01164	0.01112
19.00000	0.61875	0.01378	0.01163	0.00998
20.00000	0.61776	0.01378	0.01157	0.00997
21.00000	0.61914	0.01377	0.01131	0.00995
22.00000	0.54523	0.01376	0.01131	0.00516
23.00000	0.52314	0.01371	0.01015	0.00503
24.00000	0.48155	0.01200	0.01015	0.00502
25.00000	0.48035	0.01195	0.01014	0.00499
26.00000	0.48050	0.01190	0.01003	0.00499
27.00000	0.46324	0.01166	0.01002	0.00403
28.00000	0.41534	0.00990	0.01000	0.00400
29.00000	0.36303	0.00709	0.00988	0.00398
30.00000	0.32434	0.00700	0.00826	0.00387
31.00000	0.31665	0.00700	0.00802	0.00370
32.00000	0.29962	0.00697	0.00734	0.00370
33.00000	0.29815	0.00696	0.00733	0.00363
34.00000	0.29762	0.00695	0.00731	0.00362
35.00000	0.29308	0.00684	0.00729	0.00362
36.00000	0.29182	0.00679	0.00729	0.00362
37.00000	0.28869	0.00679	0.00710	0.00362
38.00000	0.28152	0.00678	0.00682	0.00362

39.00000	0.26967	0.00669	0.00628	0.00358
40.00000	0.26897	0.00667	0.00614	0.00357
41.00000	0.26538	0.00667	0.00595	0.00355
42.00000	0.25762	0.00667	0.00594	0.00290
43.00000	0.25394	0.00666	0.00586	0.00289
44.00000	0.25081	0.00653	0.00586	0.00285
45.00000	0.24817	0.00639	0.00585	0.00285
46.00000	0.24583	0.00637	0.00581	0.00284
47.00000	0.24397	0.00620	0.00581	0.00283
48.00000	0.23819	0.00613	0.00571	0.00274
49.00000	0.23634	0.00613	0.00564	0.00274
50.00000	0.23593	0.00613	0.00564	0.00271

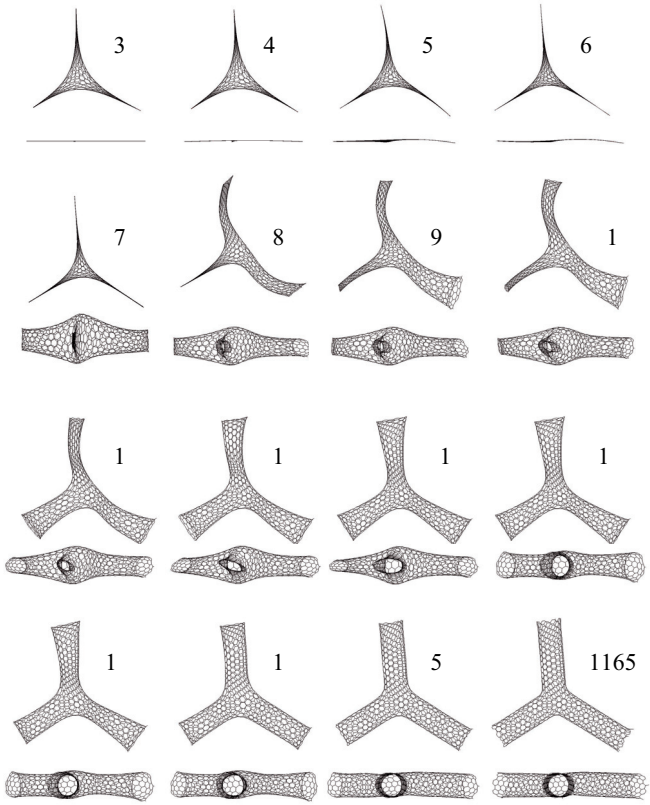

Figure 1. Top and side view of the structures obtained by the relations of Eq. (12). The number close to structures counts the eigenfunctions (m) of the Laplacian used in the summations.

Results and conclusions

The largest absolute values α_{X2}, α_{Y3} and α_{Z7}, given in Table 1, represent the coefficients of the three bi-lobal eigenvectors (Table 2). If the number of eigenfunctions (m) in Eq. (12) is smaller than 7 (the value k of the third bi-lobal eigenfunction), the picture of the structure can be described as a near planar or a curved two dimensional surface (Figure 1). The eigenvectors c_4, c_5 and c_6 are 4, 4 and 5 –lobal but they have relatively small weight in **Z** (Table 1.) Although the eigenvectors c_8, c_9, c_{10}, c_{11} and c_{12} have relatively small weight in **Z** and their lobality is from 3 to 5 they are important in eliminating the spiky features at the tube ends (Figure 1)

We can obtain a three dimensional surface only if m is greater than the order number of any bi-lobal eigenfunction. The eigenvectors c_{13} and c_{14} have significant weight in **Z**, and its influence can be seen in Figure 1. If m is greater than 16 , practically there are not significant changing in the picture of the structure. Table 3 describes, in a quantitative way the convergence of the structure. For m=7, if all of the bi-lobal eigenfunctions are used, the average difference between the position of the atoms in the calculated and the converged structure ($\left|R - R^{(c)}\right|$) is 3.59Å. For m=16 this distance changes to 0.66 Å.

We have investigated altogether 11 junctions and we obtained three-dimensional structures only if all the three bi-lobal eigenfunctions were included in the summations. We had to take into consideration some other eigenvectors for eliminating the spiky behaviours at the end of the tubes. We found in each case a value for m which provided satisfactory coordinates that can be used for initial coordinates in Molecular Mechanics calculations.

References

1. P. R. Bandaru, C. Dario, S. Jin, A. M. Rao, *Nature Mater.* **4** (2005) 663.
2. L. A. Chernozatonskii, *Phys. Lett*. **A172** (1992) 173-176.
3. L. Chico, V. H. Crespi, L. X. Benedict, S. G. Louie, M. L. Cohen, *Phys. Rev. Lett*. **76** (1996) 971-974.
4. M. Menon, D. Srivastava*, Phys. Rev. Lett.* **79** (1997) 4453-4456.
5. V. H. Crespi*, Phys. Rev.* **B58** (1998) 12671-12671.
6. G. Treboux, P. Lapstun, K. Silverbrook*, Chem. Phys. Lett*. **306** (1999) 402-406.
7. S. Melchor, N. V. Khokhriakov and S. S. Savinskii*, Mol. Eng.* **8** (1999) 315-344.
8. A. N. Andriotis, M. Menon, D. Srivastava, L. Chernozatonkii, *Appl. Phys. Lett*. **79** (2001) 266-268.

9. A. N. Andriotis, M. Menon, D. Srivastava, L. Chernozatonkii, *Phys. Rev. Lett*. **87** (2001) 066802 1-4.
10. A. N. Andriotis, M. Menon, D. Srivastava, L. Chernozatonkii, *Phys. Rev.* **B 65** (2002) 165416 1-12.
11. M. Terrones, F. Banhart, N. Grobert, J.-C. Charlier, H. Terrones, P. M. Ajayan, *Phys. Rev. Lett.* **89** (2002) 75505 1-4.
12. V. Meunier, M. B. Nardelli, J. Bernholc, T. Zacharia, J.-C. Charlier, *Appl. Phys. Lett.* **81** (2002) 5234-5234.
13. E. C. Kirby, *MATCH Commun. Math. Comput. Chem.* **48** (2003) 179-188.
14. S. Melchor, J. A. Dobado, *J. Chem. Inf. Comput. Sci.* **44** (2004) 1639-1646.
15. M. Yoon, S. Han, G. Kimm, S. B. Lee, S. Berber, E. Osawa, J. Ihm, M. Terrones, F. Banhart, J.-C. Charlier, N. Grobert, H. Terrones, P. M. Ajayan, D. Tomanek, *Phys. Rev. Lett.* **92** (2004) 75504 1-4.
16. I. Zsoldos, G. Kakuk, T. Réti, A. Szász, *Modeling Simul Mat. Sci. Eng.* **12** (2004) 1251.
17. I. Zsoldos, G. Kakuk, J. Janik, L. Pék, *Diam. Relat. Mater* **14** (2005) 763.
18. I. László, *Fullerenes, Nanotubes and Carbon Nanostructures* **13** (2005) 535.
19. I. László, *Croat. Chem. Acta* **78** (2005) 217.
20. I. László, *Croat. Chem. Acta* (2008) *accepted.*
21. I. László, *Phys. Stat. Sol. (b)* **244** (2007) 4265.
22. D.E. Manolopoulos, P.W. Fowler, *J. Chem. Phys.* **96** (1992) 7603.
23. T. Pisanski, J.S. Shawe-Taylor, *J. Chem. Inf. Comput. Sci.* **40** (2000) 567.
24. P. W. Fowler, D.E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Univ. Press, Oxford, 1995.
25. P. W. Fowler, T. Pisanski, J. Shawe-Taylor, *Molecular Graph Eigenvectors for Molecular Coordinates,* in *Graph Drawing*, DIMACS International Workshop, R. Tamassia and I. G. Tollis (Eds.), GD'94 Princeton, New Jersey, USA, October 10-12, 1994, pages 282-285.
26. I. László, A. Rassat, P.W. Fowler, A. Graovac, *Chem. Phys. Lett.* **342** (2001) 369.
27. I. László, *Carbon* **42** (2004) 983.
28. A. Graovac, D. Plavšić, M. Kaufman, T. Pisanski, E.C. Kirby, *J. Chem. Phys.* **113** (2000) 1925.
29. I. László, A. Rassat, *J. Chem. Inf. Comput. Sci.* **43** (2003) 519.
30. I. László, *The Electronic Structure of Nanotubes and the Topological Arrangements of Carbon atoms,* in *Frontiers of Multifunctional Integrated Nanosystems*, Buzaneva, E., Scharff, P. (Eds.), NATO Science Series, II. *Mathematics, Physics and Chemistry*, **152** (2004) 11.
31. I. László, *Topological Coordinates for Schlegel Diagrams of Fullerenes and Other Planar Graphs*, in *Nanostructures: Novel Architecture*, Diudea, M.V. (Ed.), Nova Science Publishers, Inc. ,New York, 2005, pp. 193.
32. M.S. Dresselhaus, G. Dresselhaus, P.C. Eklund, *Science of Fullerenes and Carbon Nanotubes*, Academic Press, San Diego, Boston, New York, 1996.